Extrapolation and interpolation of asymptotic series by self-similar approximants

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Abstract

The problem of extrapolation and interpolation of asymptotic series is considered. Several new variants of improving the accuracy of the self-similar approximants are suggested. The methods are illustrated by examples typical of chemical physics, when one is interested in finding the equation of state for a strongly interacting system. A special attention is payed to the study of the basic properties of fluctuating fluid membranes. It is shown that these properties can be well described by means of the method of self-similar approximants. For this purpose, the method has been generalized in order to give accurate predictions at infinity for a function, whose behavior is known only at the region of its variable close to zero. The obtained results for fluctuating fluid membranes are in good agreement with the known numerical data.

KEY WORDS: asymptotic series, summation of series, methods of extrapolation and interpolation, self-similar approximation theory, equations of state, fluctuating fluid membranes

1 Introduction

Asymptotic series are ubiquitous, arising in practically all realistic problems that do not allow for exact solutions but require the use of some kind of perturbation theory. The latter assumes that there exists a small parameter, such that the observable quantities of interest can be represented as series in powers of this asymptotically small parameter. However, in applications, this parameter is not negligibly small, but takes finite values. In the majority of cases, the perturbative series are divergent for the parameter finite values, corresponding to realistic systems. This is why the problem of extrapolating asymptotic series is of great importance. The problem poses the question what are the most accurate ways of extending the validity of the series, obtained for asymptotically small parameters, to the finite values of the latter. Moreover, in some cases it is necessary to extend perturbative results to the extreme limit, where the parameter tends to infinity.

The most popular techniques of extrapolating asymptotic series are based on the Padé approximants [1]. However, these have several well known shortcomings. First of all, they are not uniquely defined. For a series of a given order, there is a whole table of many Padé approximants, but there is no general recipe that would advise which of them should be preferred. The conclusion could be made if all these approximants from the table would be close to each other. Then their dispersion would define their accuracy. This, unfortunately, is a very rare case, since a rather standard situation is when the results of the approximants from the table are widely scattered, making it difficult to judge on their accuracy. Even worse, among the approximants from the table, there very often appear those that contain unreasonable poles. Then the accuracy of such approximants, strictly speaking, is not defined at all. One can, of course, neglect the approximants with the poles, calling them outliers. But, as is clear, this is a quite subjective procedure, since it may happen that the arising poles could have meaning, as is the usual case for critical phenomena. Arbitrarily rejecting some of the approximants, while keeping others, renders the whole procedure not well defined. Then one is not able to ascribe any accuracy to the obtained results. The most difficult situation is when one needs to extrapolate the perturbative series to the infinite value of the expansion parameter. In such a case, the Padé approximants cannot be used at all. In order to be specific, showing that this necessity of extrapolating the parameter to infinity does happen in realistic cases, we can mention the problem of calculating the pressure of fluctuating fluid membranes.

Different types of membranes are rather frequent structures in chemical and biological systems [2–6]. The membrane thermal fluctuations between two hard walls are often described by field theory. An important class of membranes are fluid membranes, whose constituent molecules are able to move within them. The fluctuations are controlled by their bending rigidity.

When applying field theory to the description of membranes, one encounters the following problem. First, to proceed in calculations, one replaces the hard walls by a smooth potential of a finite stiffness, which, in dimensionless units, can be denoted as g. Then, one is able to proceed by invoking perturbation theory in powers of g. However, to return back to the sought case of rigid walls, one needs to set $g \to \infty$. Thus, the problem arises how from an expansion in powers of small $g \to 0$ one could extract information on the quantities of interest for large $g \to \infty$? The standard resummation techniques, such as

Borel or Padé [6] could help in extending asymptotic series in small $g \to 0$ to finite values of g, but these techniques are not applicable for the limit of $g \to \infty$.

The problem of extending a function f(g), which is known only for asymptotically small $g \to 0$, to the whole region of g, including the limit $g \to \infty$, can be solved by the optimized perturbation theory, advanced in Ref. [7]. This theory has been successfully applied to a variety of problems, as can be inferred from the review-type articles [8,9] and references therein. The pivotal idea of the optimized perturbation theory [7] is to introduce in the calculational process control functions defined by optimization conditions. As a result, a function f(g), known only for small $g \to 0$, can be extrapolated to the whole region of q, including the limit $q \to \infty$. There exist three main ways of introducing control functions. One way is to include in the initial approximation trial parameters that are transformed, by means of the optimization conditions, into control functions at each step of perturbation theory. Another way is to introduce control functions in the process of accomplishing a perturbative or iterative scheme, for instance, by defining the cutoffs of integrals or introducing regularization masses, which are then to be transformed into control functions. The third way is to derive, first, an asymptotic series in powers of a small parameter or variable and then to reorganize the derived series by means of a change of variables, with control functions included in this variable transformation. Various examples of introducing control functions can be found in literature [10–30] (see also the review articles [8,9]).

The optimized perturbation theory has been applied to fluid membranes in several papers. The most accurate results have been obtained by Kastening [31], whose calculations are based on the sixth-order perturbation theory, with introducing control functions by means of the Kleinert change of variables [32]. This method requires rather heavy numerical calculations. Also, the Kastening result [31] slightly deviates from the Monte Carlo [33] simulations for this problem.

The aim of the present paper is to reconsider the general problem of extrapolating asymptotic series in order to find an accurate and simple way of accomplishing such an extrapolation. We also consider the case when the behavior at infinity is known, which then becomes the problem of an accurate interpolation. We pay a special attention to developing simple methods for obtaining the limit $f(\infty)$ at $g \to \infty$ from the asymptotic expansion of f(g) at $g \to 0$. To illustrate the methods, we apply them to several problems, which yield the series, whose mathematical structure is typical for many real situations in chemical physics. At the end, we apply these methods to considering the problem of fluid fluctuating membranes.

The method we aim at developing is based on the self-similar approximation theory [34–41] in the variant involving the self-similar root approximants [42–44] and self-similar factor approximants [45–49]. This approach has been applied to variety of problems, providing high accuracy and at the same time being quite simple [42–49]. It was shown to be essentially more accurate than the use of Padé approximants [42–52]. However, in some cases, when the self-similar approximants were directly applied for solving the problems involving the limit of $g \to \infty$, the results were not satisfactory. Our aim now is to generalize the method of self-similar approximants so that it would provide good accuracy for the limiting value of $f(\infty)$ at $g \to \infty$. Then we apply the method to solving several problems requiring the construction of the equations of state for strongly

interacting systems. Among them, we study the problem of fluctuating fluid membranes and demonstrate that the newly developed methods provide good accuracy by comparing our results with the known numerical calculations.

2 Factor and root approximants

First, we need to recall the method of self-similar factor and root approximants [42–52], which we are going to improve. Suppose, we are interested in the behavior of a real function f(g) of a real variable g. And let us assume that this function is defined by so complicated equations that the sole thing we are able to find is the property of the function at asymptotically small g, where

$$f(g) \simeq f_k(g) \qquad (g \to 0)$$
 (1)

is approximated by the series

$$f_k(g) = f_0(g) \sum_{n=0}^k a_n g^n ,$$
 (2)

in which $f_0(g)$ is a form that cannot be expanded in powers of g. Without the loss of generality, we can set $a_0 = 1$, since any a_0 not equal to one can be incorporated into $f_0(g)$.

Series (2), which are valid for $g \to 0$, can be extrapolated to the region g > 0 by means of the self-similar factor approximants [45–49] having the form

$$f_k^*(g) = f_0(g) \prod_{i=1}^{N_k} (1 + A_i g)^{n_i},$$
 (3)

where

$$N_k = \begin{cases} k/2, & k = 2, 4, \dots \\ (k+1)/2, & k = 3, 5, \dots \end{cases}$$
 (4)

The parameters A_i and n_i are defined by the re-expansion procedure, when the k-th order approximant (3) is expanded in powers of g up to the k-th order as

$$f_k^*(g) \simeq f_0(g) \sum_{n=0}^k a_n^* g^n ,$$
 (5)

where $a_n^* = a_n^*(\{A_i\}, \{n_i\})$. Then expansions (2) and (5) are compared, with equating the same-order terms

$$a_n^*(\{A_i\}, \{n_i\}) = a_n$$
 (6)

This way is also called the accuracy-through-order procedure.

In order to give an explicit representation of Eqs. (6), it is convenient to equate the logarithms

$$\ln f_k^*(g) \simeq \ln f_k(g) \qquad (g \to 0) , \qquad (7)$$

which, taking into account form (3), yields

$$\sum_{i=1}^{N_k} n_i \ln(1 + A_i g) \simeq \ln \sum_{m=0}^k a_m g^m .$$
 (8)

Expanding here

$$\ln(1 + A_i g) = \sum_{m=1}^{\infty} \frac{(-1)^{m-1}}{m} (A_i g)^m,$$

we come to the equations

$$\sum_{i=1}^{N_k} n_i A_i^n = B_n \qquad (n = 1, 2, \dots, k) , \qquad (9)$$

in which

$$B_n = \frac{(-1)^{n-1}}{(n-1)!} \lim_{g \to 0} \frac{d^n}{dg^n} \ln \left(\sum_{m=0}^n a_m g^m \right) . \tag{10}$$

The system of equations (9) contains k equations. When k is even, system (9) defines all k/2 parameters A_i and k/2 parameters n_i . When k is odd, then there are k+1 parameters, (k+1)/2 parameters A_i , and (k+1)/2 parameters n_i . Then the system (9) is complemented by the condition $A_1 = 1$ following from the scaling arguments [47,48]. Thus, the re-expansion procedure completely defines all parameters of the self-similar approximant (3). It may happen, though it is a rather rare case, that Eqs. (9), for some order k, do not have solutions. Then one just needs to proceed to the higher orders of the series. But it is important to stress that for each given order k the factor approximants are uniquely defined. So, when Eqs. (9) possess solutions, these solutions are unique.

The described above method allows for the extrapolation of a series for a small $g \to 0$ to the finite values of g. In some cases, there can exist additional information on the behavior of the function at asymptotically large g,

$$f(g) \simeq f_p(g) \qquad (g \to \infty) ,$$
 (11)

so that

$$f_p(g) = \sum_{j=1}^p b_j g^{\alpha_j} \qquad (\alpha_j > \alpha_{j+1}) , \qquad (12)$$

with the powers α_j in the descending order. In that case, we have the problem of interpolation between small $g \to 0$ and large $g \to \infty$. Suppose that $f_0(g)$ at large g behaves as

$$f_0(g) \simeq Ag^{\alpha} \qquad (g \to \infty) \ .$$
 (13)

Then, in order that the factor approximant (3) would satisfy the limiting form (12), we need to set

$$A \prod_{i=1}^{N_k} A_i^{n_i} = b_1 \qquad \alpha + \sum_{i=1}^{N_k} n_i = \alpha_1 . \tag{14}$$

This type of the interpolating factor approximant, employing k terms from the small-variable expansion and one limiting term from the large-variable behavior, will be denoted

as $f_{k+1}^*(g)$. In the following sections, we develop alternative methods of interpolation, improving the accuracy of the factor approximants

The problem of interpolation can also be conveniently solved by involving the self-similar root approximants [42-44], having the form

$$R_p^*(g) = f_0(g) \left(\dots \left((1 + A_1 g)^{n_1} + A_2 g^2 \right)^{n_2} + \dots + A_p g^p \right)^{n_p} . \tag{15}$$

The parameters A_i and n_i are defined by the large-variable expansion (12). Again, it is important to emphasize that this definition is unique [9]. If, instead, we try to define the parameters of a k-order root approximant by the accuracy-through-order procedure, expanding Eq. (15) in powers of g and equating the resulting expansion with Eq. (2), then we confront the problem of nonuniqueness of solutions for the sought parameters [50]. In the following sections, we shall suggest a way of solving this problem. It is worth noting that the regions of small g and large g can be easily interchanged by the change of the variable g to 1/g.

3 Problem of self-similar interpolation

One of the well known difficulties in dealing with asymptotic series occurs when the number of their terms is small, which does not allow one to construct higher order approximants. In the present section, we suggest a way of overcoming this difficulty. The method, we advance, reminds the learning algorithms used in statistical learning [53]. The idea is as follows. Suppose we have k terms a_k of the small-variable expansion and the limiting form of the large-variable behavior. Interpolating from the right to left, that is, considering the variable 1/g, we construct the corresponding self-similar approximant, say, the root approximant $R_k^*(g)$. Then we expand the latter in powers of g up to the (k+1)-order, obtaining an additional term a_{k+1}^* . Using the new expansion, we define the approximant $R_{k+1}^*(g)$. Expanding this up to the (k+2)-order, we find the (k+2)-order term a_{k+2}^* . Then, we construct the approximant $R_{k+2}^*(g)$, and so on. Thus, each approximant defines the higher-order term of the small-g expansion. Of course, this procedure can work only when the sought function pertains to the class of monotonic functions and the interpolation problem is considered. Below, we illustrate the method by examples where one is interested in finding the equations of state.

3.1 Fröhlich optical polaron

Let us consider the problem of the optical polaron, being interested in finding its energy e(g) as a function of the coupling parameter g. It is common to employ the dimensionless notations for these quantities, which we use in what follows. The small-g expansion and the large-g limit can be found in the review article [54]. For the small-g expansion, one has

$$e(g) \simeq a_1 g + a_2 g^2 + a_3 g^3 \qquad (g \to 0) ,$$
 (16)

with the coefficients

$$a_1 = -1$$
, $a_2 = -1.591962 \times 10^{-2}$, $a_3 = -0.806070 \times 10^{-3}$,

While the large-g behavior is given by the Miyake limit

$$e(g) \simeq Bg^2 + O(1) \qquad (g \to \infty) , \qquad (17)$$

where B = -0.108513.

Following the procedure described above, we derive the coefficients

$$a_4^* = -5.014168 \times 10^{-5}$$
, $a_5^* = -3.312472 \times 10^{-6}$.

Using these and interpolating from the right to left, with the variable $1/g^2$, we construct the root approximant

$$R_4^*(g) = Bg^2 \left(\left(\left(\left(1 + \frac{A_1}{g^2} \right)^{n_1} + \frac{A_2}{g^4} \right)^{n_2} + \frac{A_3}{g^6} \right)^{n_3} + \frac{A_4}{g^8} \right)^{n_4}, \tag{18}$$

where

$$A_1 = 64.163254,$$
 $A_2 = 7.001856 \times 10^3,$ $A_3 = 7.026125 \times 10^5,$ $A_4 = 5.201706 \times 10^7,$ $n_1 = \frac{3}{2},$ $n_2 = \frac{5}{4},$ $n_3 = \frac{7}{6},$ $n_4 = \frac{1}{8},$

and the root approximant

$$R_5^*(g) = Bg^2 \left(\left(\left(\left(\left(\left(1 + \frac{A_1}{g^2} \right)^{n_1} + \frac{A_2}{g^4} \right)^{n_2} + \frac{A_3}{g^6} \right)^{n_3} + \frac{A_4}{g^8} \right)^{n_4} + \frac{A_5}{g^{10}} \right)^{n_5}, \quad (19)$$

with the coefficients

$$A_1 = 68.38553,$$
 $A_2 = 7.742967 \times 10^3,$ $A_3 = 8.213401 \times 10^5,$ $A_4 = 7.313112 \times 10^7,$ $A_5 = 4.417553 \times 10^9,$ $n_1 = \frac{3}{2},$ $n_2 = \frac{5}{4},$ $n_3 = \frac{7}{6},$ $n_4 = \frac{9}{8},$ $n_5 = \frac{1}{10}.$

The accuracy of these approximants can be checked by comparing them with the results of the Monte Carlo simulations [54] accomplished for the region of $g \in [1, 15]$. In all this region, the approximant (19) has the percentage error less than 1%. The maximal error of -1% occurs at g=10, where this error is comparable with the Feynman variational calculations [55]. But for all other values of g in the considered interval, the accuracy of approximant (19) is better than the Feynman results. Comparing the accuracy of the approximants $R_3^*(g)$, $R_4^*(g)$, and $R_5^*(g)$, we observe numerical convergence. For instance, the maximal percentage error of $R_3^*(g)$ is 1.5% at g=10.

3.2 One-dimensional Bose gas

Let us now consider the ground-state energy e(g) of the Lieb-Liniger model [56] as a function of the coupling parameter g, again using dimensionless units. The weak-coupling expansion can be written [57,58] as

$$e(g) \simeq g + a_3 g^{3/2} + a_4 g^2 + a_5 g^{5/2}$$
, (20)

with the coefficients

$$a_3 = -0.424413$$
, $a_4 = 0.065352$, $a_5 = -0.017201$.

For strong coupling, we have the Tonks-Girardeau limit

$$e(g) \simeq \frac{\pi^2}{3} + O\left(\frac{1}{g}\right) \qquad (g \to \infty) \ .$$
 (21)

Following the procedure, described at the beginning of this section, we find

$$a_6^* = 5.153629 \times 10^{-3}$$
.

Then we construct the root approximants of different orders, interpolating from the right to left, with the variable 1/g, and compare their accuracy with numerical data [58]. The approximant $R_5^*(g)$ has the maximal, with respect to the whole range of $g \in [0, \infty)$, error of 3.4% at g = 6. The maximal error of $R_6^*(g)$ is 1.75% at g = 10. The best approximant is obtained using the coefficients a_3 and a_4 of expansion (20) and the three terms of the strong coupling limit that can be written [57,58] as

$$e(g) \simeq \frac{\pi^2}{3} \left(1 - \frac{4}{g} + \frac{12}{g^2} \right) \qquad (g \to \infty) .$$
 (22)

The corresponding root approximant is

$$R_{4+3}^*(g) = \frac{\pi^2}{3} \left(\left(\left(\left(\left(\left(1 + \frac{A_1}{g} \right)^{n_1} + \frac{A_2}{g^2} \right)^{n_2} + \frac{A_3}{g^3} \right)^{n_3} + \frac{A_4}{g^4} \right)^{n_4} + \frac{A_5}{g^5} \right)^{n_5}, \quad (23)$$

where

$$A_1 = 8.126984,$$
 $A_2 = 37.345427,$ $A_3 = 164.914098,$ $A_4 = 388.171278,$ $A_5 = 385.382911,$ $n_1 = \frac{3}{2},$ $n_2 = \frac{5}{4},$ $n_3 = \frac{7}{6},$ $n_4 = \frac{9}{8},$ $n_5 = \frac{1}{5}.$

This approximant (23) provides a very high accuracy in the whole range of $g \in [0, \infty)$, having the maximal error of only 0.023% at g = 6. Therefore, expression (23) can be employed as an analytical representation for the ground-state energy of the Lieb-Liniger gas.

3.3 Diluted Fermi gas

Let us now turn to defining the ground-state energy of the spin 1/2 Fermi gas with attractive interactions, corresponding to the negative scattering length a_s . The ground-state energy e(g) can be written [59] as an asymptotic expansion in powers of the dimensionless parameter $g = |k_F a_s|$, where k_F is the Fermi wave vector,

$$e(g) \simeq a_0 + a_1 g + a_2 g^2 + a_3 g^3 + a_4 g^4$$
. (24)

Here $g \to 0$ and

$$a_0 = \frac{3}{10}$$
, $a_1 = -\frac{1}{3\pi}$, $a_2 = 0.055661$,
 $a_3 = -0.00914$, $a_4 = -0.018604$.

In the unitary limit [60,61], when $g \to \infty$, numerical calculations [62] yield

$$\lim_{g \to \infty} e(g) = 0.132 \ . \tag{25}$$

We construct the self-similar approximants of different orders and compare their accuracy with Monte Carlo simulations [63]. The factor approximant $f_{3+1}^*(g)$ turns out to be analogous to the diagonal [2/2] Padé approximant [64]. However, the root approximant $R_3^*(g)$ is essentially more accurate. The factor approximant $f_{4+1}^*(g)$ displays the same accuracy as $R_3^*(g)$. The maximal percentage error of the latter two approximants in the interval of $g \in [0, 5]$ is only about 0.2%.

4 Problem of self-similar extrapolation

The problem of extrapolation of asymptotic series is much more difficult than that of their interpolation. In the latter case, the large-variable limit is given, while in the former case, this limit is not known. And often, it is exactly the limiting behavior at large variable, which is of the most interest. In the present section, we suggest new variants of constructing the self-similar approximants in the extrapolation problem and illustrate these methods by the model whose mathematical structure is typical of the variety of physical and chemical systems.

4.1 Iterated root approximants

The extrapolation of asymptotic series can be done by means of the self-similar factor approximants. But, as is mentioned in Sec.2, if we try to accomplish the extrapolation by using the root approximants, we encounter the problem of nonuniqueness of defining their parameters by the accuracy-through-order procedure. To overcome this problem, we suggest to use the iteration method, by keeping the fixed lower-order parameters when constructing the higher-order approximants. Then all parameters of the root approximants can be uniquely defined.

To be concrete, let us consider the anharmonic-oscillator model with the Hamiltonian

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 + gx^4, \qquad (26)$$

where $x \in (-\infty, \infty)$ and the dimensionless coupling parameter is positive, being in the region $g \in [0, \infty)$. The weak-coupling expansion for the ground-state energy [65] reads as

$$e(g) \simeq a_0 + a_1 g + a_2 g^2 + a_3 g^3 + a_4 g^4 + a_5 g^5 + a_6 g^6 + a_7 g^7$$
, (27)

with the coefficients

$$a_0 = \frac{1}{2}, \qquad a_1 = \frac{3}{4}, \qquad a_2 = -2.625,$$

$$a_3 = 20.8125, \qquad a_4 = -241.2890625, \qquad a_5 = 3580.98046875,$$

$$a_6 = -63982.8134766, \qquad a_7 = 1329733.72705.$$

Our aim is to extrapolate the weak-coupling expansion (27), valid for asymptotically small $g \to 0$, to the region of finite values of g. And we shall pay a special attention to the behavior of the extrapolated energy at large $g \to \infty$, comparing it with the known asymptotic form

$$e(g) \simeq 0.667986g^{1/3} \qquad (g \to \infty) \ .$$
 (28)

The iteration method for constructing the uniquely defined root approximants is elucidated in the following forms extrapolating the asymptotic expansion (27) to finite values of g. We start with the lowest approximant

$$R_2^*(g) = \frac{1}{2} (1 + A_1 g)^{n_1} , \qquad (29)$$

in which

$$A_1 = 8.5, \qquad n_1 = 0.176.$$

The next-order approximant is

$$R_4^*(g) = \frac{1}{2} \left((1 + A_1 g)^{n_2} + A_2 g^3 \right)^{n_3} , \qquad (30)$$

with the same A_1 and

$$A_2 = 227.719, n_2 = \frac{n_1}{n_3} = 2.771, n_3 = 0.064.$$

The next approximant

$$R_6^*(g) = \frac{1}{2} \left(\left((1 + A_1 g)^{n_2} + A_2 g^3 \right)^{n_4} + A_3 g^5 \right)^{n_5} , \tag{31}$$

contains the same A_1 , n_2 , and A_2 , with

$$A_3 = 3.827 \times 10^4$$
, $n_4 = \frac{n_3}{n_5} = 2.001$, $n_5 = 0.032$.

We shall compare the strong-coupling behavior of these root approximants with the exact limiting form (28) and with the factor approximant

$$f_6^*(g) = \frac{1}{2} (1 + B_1 g)^{m_1} (1 + B_2 g)^{m_2} (1 + B_3 g)^{m_3} , \qquad (32)$$

in which

$$B_1 = 26.74018, \qquad B_2 = 12.46882, \qquad B_3 = 3.83804,$$
 $m_1 = 1.80165 \times 10^{-3}, \qquad m_2 = 0.05473, \qquad m_3 = 0.20047.$

The strong-coupling behavior of the root approximants (29) to (31) is

$$R_2^*(g) \simeq \frac{1}{2} (A_1 g)^{n_1} , \qquad R_4^*(g) \simeq \frac{1}{2} \left(A_2 g^3 \right)^{n_3} , \qquad R_6^*(g) \simeq \frac{1}{2} \left(A_2 g^3 \right)^{n_4 n_5} .$$
 (33)

While the factor approximant (32), as $g \to \infty$, gives

$$f_6^*(g) \simeq \frac{1}{2} B_1^{m_1} B_2^{m_2} B_3^{m_3} g^{m_1 + m_2 + m_3}$$
 (34)

Substituting here the corresponding values of the parameters yields

$$R_2^*(g) \simeq 0.728698g^{0.176} , \qquad R_4^*(g) \simeq 0.707691g^{0.192} ,$$

 $R_6^*(g) \simeq 0.707814g^{0.192} , \qquad f_6^*(g) \simeq 0.756157g^{0.257} .$ (35)

Comparing these expressions with the exact asymptotic form (28), we see that the amplitudes of the root approximants provide slightly better extrapolation than the factor approximant, however this difference is not essential, all amplitudes being defined with an error of about 10%. In many cases, the most important quantity that is required to be found from the extrapolation procedure is the power of g in the limit of $g \to \infty$. Equation (35) shows that the best extrapolation of the power is provided by the factor approximant, whose error is about 20%, while the root approximants have a twice larger error. The accuracy can be improved by defining the higher-order approximants.

In the present section we demonstrated the application of the method of iterated root approximants to the problem of calculating the ground-state energy of the anharmonic oscillator. This method works well for other problems too. For example, we have constructed the iterated root approximants for the problem of the one-dimensional Bose gas of Sec. 3.2. The root approximant $R_6^*(g)$, extrapolated from the left to right, gives the energy $e(\infty)$, as $t \to \infty$, equal to 3.292, which is very close to the Tonks-Girardeau limit $\pi^2/3$. We have also considered the iterated root approximants for the problem of the diluted Fermi gas of Sec. 3.3. Extrapolating the ground-state energy from small $g \to \infty$ to the strong-coupling limit $g \to \infty$ for $R_4^*(g)$ provides an accuracy within the maximal error of order 10%.

4.2 Odd factor approximants

In the definition of the factor approximants of odd orders, there is a necessity of prescribing the value of one of the parameters, say A_1 , in the general form (3). According to the scaling arguments [47,48], this parameter can be set to one. Here we suggest one more variant of setting this parameter by defining it as a_1/a_0 .

Keeping in mind the same problem of extrapolating the ground-state energy of the anharmonic oscillator with Hamiltonian (26), we need to compare the accuracy of the corresponding factor approximants. The standard form is

$$f_5^*(g) = \frac{1}{2}(1+g)^{n_1}(1+A_2g)^{n_2}(1+A_3g)^{n_3} , \qquad (36)$$

where

$$A_2 = 21.86082, \qquad A_3 = 8.48018,$$

$$n_1 = 0.27622, \qquad n_2 = 7.16531 \times 10^{-3}, \qquad n_3 = 0.12584 \; .$$

In the strong-coupling limit, this gives

$$f_5^*(g) \simeq 0.669 g^{0.409} \qquad (g \to \infty) \ . \tag{37}$$

Another variant of the factor approximant reads as

$$f_5^{**}(g) = \frac{1}{2} \left(1 + \frac{a_1}{a_0} g \right)^{n_1} (1 + A_2 g)^{n_2} (1 + A_3 g)^{n_3} , \qquad (38)$$

with the parameters

$$A_2 = 22.16875, \qquad A_3 = 8.83021,$$

$$n_1 = 0.2212, \qquad n_2 = 6.55016 \times 10^{-3}, \qquad n_3 = 0.11585.$$

Now, the strong-coupling limit becomes

$$f_5^{**}(g) = 0.718g^{0.344} \qquad (g \to \infty) .$$
 (39)

As is seen, the first form (36) extrapolates better the amplitude, while the second variant gives a better extrapolation of the power. Generally, there is no appriori preference for choosing this or that form, which, actually, is in agreement with the scaling arguments [47,48].

4.3 Weighted factor-root approximants

One more possibility is to construct the weighted approximants defined as the linear combination of the factor and root approximants of the form

$$W_k^*(g) = \lambda f_k^*(g) + (1 - \lambda) R_k^*(g) , \qquad (40)$$

with all parameters determined from the accuracy-through-order matching. The accuracy of such weighted approximants can be essentially improved. A more general way of constructing average values for an ensemble of approximants was considered in Ref. [66]

5 Problem of extrapolation to infinity

The self-similar factor approximants (3) extrapolate the asymptotic series (2), valid for small $g \to 0$, to the region of finite g > 0. These approximants, as has been shown by numerous examples [45–49], provide for finite, even rather large, g very good approximations, essentially more accurate than Padé approximants.

But the problem, we face now, is to extrapolate series (2) not simply to finite or large g, but to find the limit $f(\infty)$ at $g \to \infty$, of course, assuming that this limit exists, so that

$$f(\infty) = \lim_{g \to \infty} f(g) = const. \tag{41}$$

By requiring that the limit

$$f_k^*(\infty) = \lim_{g \to \infty} f_k^*(g) = const \tag{42}$$

would also exist, in view of Eq. (3), we come to the condition

$$\lim_{g \to \infty} f_0(g) \prod_{i=1}^{N_k} (A_i g)^{n_i} = const .$$
 (43)

Let, for concreteness, the behavior of $f_0(g)$ at large g be $f_0(g) \simeq Ag^{\alpha}$ $(g \to \infty)$, as in Eq. (13). Then, for condition (43) to hold, it is necessary and sufficient that

$$\alpha + \sum_{i=1}^{N_k} n_i = 0 \ . \tag{44}$$

Therefore the value of approximant (3), given by

$$f_k^*(\infty) = A \prod_{i=1}^{N_k} A_i^{n_i} , \qquad (45)$$

provides the approximation for the sought limit $f(\infty)$.

This method of defining the limit $f_k^*(\infty)$ at $g \to \infty$ by imposing the restriction (44) on the powers of the approximant (3) is very simple. However, as has been analyzed in Refs. [45,46], its accuracy is not high. In the following section, we suggest another method, whose high accuracy will be illustrated by calculating the pressure of fluctuating membranes.

6 Method of variable transformation

Instead of considering the limit $f(\infty)$ at $g \to \infty$, it is convenient to make the change of variables

$$g = g(z) , \qquad z = z(g) , \qquad (46)$$

such that

$$\lim_{g \to \infty} z(g) = 1. \tag{47}$$

Then, for the function

$$F(z) \equiv f(g(z)) , \qquad (48)$$

the sought limit is given by

$$F(1) = f(\infty) \tag{49}$$

at z=1.

With the change of variables (46), the series (2) become

$$f_k(g(z)) \cong F_k(z) \qquad (z \to 0) ,$$
 (50)

where

$$F_k(z) = F_0(z) \sum_{n=0}^k b_n z^n$$
 (51)

is an expansion in powers of z up to the k-th order, with the coefficients $b_0 = 1$ and $b_n = b_n(a_1, a_2, \ldots, a_k)$ defined through the coefficients a_n of series (2). Then, constructing for sum (51) the factor approximant $F_k^*(z)$, we obtain the approximation $F_k^*(1)$ for the sought limit $f(\infty)$.

In order to specify transformation (46), we assume the following natural properties. According to condition (47), it should be that $z \to 1$ as $g \to \infty$. If the asymptotic behavior of the sought function is

$$f(g) \simeq f(\infty) \left(1 + \frac{C_1}{g^{\omega}} \right) \qquad (g \to \infty) ,$$
 (52)

we require that transform (48) be

$$F(z) \simeq F(1)[1 + C_2(1-z)] \qquad (z \to 1) ,$$
 (53)

where C_1 and C_2 are constants and $\omega > 0$. And, in agreement with Eqs. (50) and (51), we assume that $z \to 0$ as $g \to 0$, so that

$$g(z) \simeq \lambda z \qquad (z \to 0) , \tag{54}$$

with a scaling parameter $\lambda > 0$.

Comparing Eqs. (52) and (53) requires that

$$\frac{C_1}{g^{\omega}} \simeq C_2(1-z) \qquad (z \to 1) , \qquad (55)$$

where we take into account that $f(\infty) = F(1)$. This yields

$$g(z) \simeq \frac{C_3}{(1-z)^{1/\omega}} \qquad (z \to 1) ,$$
 (56)

where $C_3 \equiv (C_1/C_2)^{1/\omega}$. The interpolation between limits (54) and (56) can be done by using the self-similar factor approximants [45–50], which results in the form

$$g(z) = \frac{\lambda z}{(1-z)^{1/\omega}} \ . \tag{57}$$

Thus, we obtain an explicit expression for the change of variables (46). For simplicity, we set in what follows the scaling parameter $\lambda = 1$.

But we need yet to define the exponent ω . For this purpose, we introduce the function

$$\beta(g) \equiv \frac{d \ln f(g)}{d \ln g} = \frac{g}{f(g)} \frac{d f(g)}{d g}. \tag{58}$$

It is easy to notice that, if f(g) enjoys the asymptotic behavior (52), then the function (58) behaves as

$$\beta(g) \simeq -\omega C_1 g^{-\omega} \qquad (g \to \infty) \ .$$
 (59)

Therefore, the exponent ω is defined as

$$\omega = -\lim_{g \to \infty} \frac{\ln |\beta(g)|}{\ln q} \,. \tag{60}$$

This procedure is to be accomplished in each approximation order. That is, for the given $f_k(g)$, defined in Eq. (2), we write

$$\beta_k(g) = \frac{d \ln f_k(g)}{d \ln q} \tag{61}$$

and expand this in powers of g, getting

$$\beta_k(g) = \beta_0(g) \sum_{n=0}^k c_n g^n ,$$
 (62)

with the coefficients $c_0 = 1$ and $c_n = c_n(a_1, a_2, ..., a_k)$ prescribed by the coefficients a_n . Then, we construct the factor approximant

$$\beta_k^*(g) = \beta_0(g) \prod_{i=1}^{N_k} (1 + D_i g)^{m_i}$$
(63)

for series (62). From here, considering the limit $g \to \infty$, we get

$$\omega_k = -\lim_{g \to \infty} \frac{\ln |\beta_k^*(g)|}{\ln g} , \qquad (64)$$

in analogy with Eq. (60).

Let, for example, the first factor in Eq. (63) behave as

$$\beta_0(g) \simeq Bg^{\gamma} \qquad (g \to \infty) \ . \tag{65}$$

Then approximant (63), at large $g \to \infty$, is

$$\beta_k(g) \simeq Bg^{\gamma} \prod_{i=1}^{N_k} (D_i g)^{m_i} \qquad (g \to \infty) . \tag{66}$$

As a result, Eq. (64) gives

$$\omega_k = -\left(\gamma + \sum_{i=1}^{N_k} m_i\right) . {(67)}$$

To summarize, the calculational scheme is as follows. For a given series (2), we find the function (62) and construct its factor approximant (63), which provides us with the exponent (67):

$$f_k(g) \to \beta_k(g) \to \beta_k^*(g) \to \omega_k$$
 (68)

Then, making the change of the variable

$$g = \frac{z}{(1-z)^{1/\omega_k}} \,, \tag{69}$$

from $f_k(g)$, we obtain expression (51). Constructing for the latter the factor approximant $F_k^*(z)$, we come to the value $F_k^*(1)$ approximating the sought limit $f(\infty)$:

$$F_k(z) \to F_k^*(z) \to F_k^*(1)$$
 (70)

When constructing the self-similar approximant $F_k^*(z)$, we need to solve the system of equations (9). Sometimes, though rare, it may happen that Eqs. (9), for some k, have no solutions which would yield real self-similar factor approximants. In that case, for $F_k^*(z)$ we take the arithmetic average of its neighbors $F_k^* = (F_{k-1}^* + F_{k+1}^*)/2$. In practical calculations, one always deals with the approximation orders k = 1, 2, ..., K up to a finite maximal order K. Then the final answer for the set of F_k^* is given by the average of two last terms $(F_K^* + F_{K-1}^*)/2$. The scheme, formulated in the present Section, will be applied to studying the properties of fluctuating membranes in the following Sections.

7 Energy of one-dimensional membrane

A cartoon of a membrane is a one-dimensional string oscillating between two rigid walls. This model, to our knowledge, was suggested by Edwards [67] and later considered in many articles [2–6,68]. It has been shown that calculating the free energy of the string is equivalent to finding the ground-state energy of a quantum particle in a one-dimensional box. Replacing the rigid walls by a soft potential, characterized by a finite stiffness g, and employing perturbation theory with respect to g yields the series

$$E_k(g) = \frac{\pi^2}{8g^2} \sum_{n=0}^k a_n g^n$$
 (71)

for the particle ground-state energy E(g), with the coefficients

$$a_0 = 1$$
, $a_1 = \frac{1}{4}$, $a_2 = \frac{1}{32}$, $a_3 = \frac{1}{512}$, $a_4 = 0$, $a_5 = -\frac{1}{131072}$, $a_6 = 0$, $a_7 = \frac{1}{16777216}$, $a_8 = 0$, $a_9 = -\frac{5}{8589934592}$,

and so on.

The series (71) are obtained for the asymptotically small $g \to 0$. But, in order to pass to the case of hard walls, one has to consider the limit $g \to \infty$, with $E(\infty)$ being the sought value. Fortunately, the one-dimensional case allows for an explicit solution [67–69] giving

$$E(g) = \frac{\pi^2}{8g^2} \left(1 + \frac{g^2}{32} + \frac{g}{4} \sqrt{1 + \frac{g^2}{64}} \right) , \qquad (72)$$

from where

$$E(\infty) = \frac{\pi^2}{128} = 0.077106 \ . \tag{73}$$

This makes it possible to evaluate the accuracy of the self-similar approximants $E_k^*(\infty)$ with respect to the exact limit (73).

We also wish to compare the accuracy of the two methods described above. First, we use the direct method by imposing restriction (44). To this end, we construct the factor approximants

$$E_k^*(g) = \frac{\pi^2}{8g^2} \prod_{i=1}^{N_k} (1 + A_i g)^{n_i}$$
 (74)

for series (71). Imposing the power restriction condition (44), we have

$$\sum_{i=1}^{N_k} n_i = 2 \ . \tag{75}$$

So that the sought limit is given by

$$E_k^*(\infty) = \frac{\pi^2}{8} \prod_{i=1}^{N_k} A_i^{n_i} , \qquad (76)$$

according to Eq. (45). The accuracy of approximants (76) is characterized by the percentage errors

$$\varepsilon(E_k^*) \equiv \frac{E_k^*(\infty) - E(\infty)}{E(\infty)} \cdot 100\% \tag{77}$$

with respect to the exact value (73).

Another way is to follow the method of Sec. 6. Then we find the function (61), with expansion (62), which reads as

$$\beta_k(g) = -2\sum_{n=0}^k c_n g^n \,, \tag{78}$$

with the coefficients

$$c_0 = 1$$
, $c_1 = -\frac{1}{8}$, $c_2 = 0$, $c_3 = \frac{1}{1024}$,
 $c_4 = 0$, $c_5 = -\frac{3}{262144}$, $c_6 = 0$, $c_7 = \frac{5}{33554432}$,
 $c_8 = 0$, $c_9 = -\frac{35}{17179869184}$,

etc.

Constructing the factor approximants (63) for series (78), we find

$$\beta_k^*(g) = \frac{2g}{\sqrt{64 + g^2}} - 2 \tag{79}$$

for all $k \geq 4$. Therefore, the exponent (34) is

$$\omega_k = 2 \qquad (k \ge 4) \ . \tag{80}$$

Hence, transformation (69) becomes

$$g = \frac{z}{\sqrt{1-z}} \,. \tag{81}$$

Using g = g(z), given by Eq. (81), we get

$$F(z) \equiv E(g(z)) , \qquad (82)$$

similarly to Eq. (48). And the related series (81) acquire the form

$$F_k(z) = \frac{\pi^2}{8z^2} \sum_{n=0}^k b_n z^n , \qquad (83)$$

with the coefficients

$$b_0 = 1 , \qquad b_1 = -\frac{3}{4} , \qquad b_2 = -\frac{3}{32} , \qquad b_3 = -\frac{15}{512} ,$$

$$b_4 = -\frac{15}{1024} , \qquad b_5 = -\frac{1185}{131072} , \qquad b_6 = -\frac{1635}{262144} ,$$

$$b_7 = -\frac{77295}{16777216} , \qquad b_8 = -\frac{119595}{33554432} , \qquad b_9 = -\frac{24489285}{8589934592} ,$$

and so on.

Then, for series (83), we find the factor approximants

$$F_k^*(z) = \frac{\pi^2}{8z^2} \prod_{i=1}^{N_k} (1 + B_i z)^{n_i} , \qquad (84)$$

whose values $F_k^*(1)$ approximate the sought limit $E(\infty)$. The accuracy of $F_k^*(1)$ is characterized by the percentage errors

$$\varepsilon(F_k^*) \equiv \frac{F_k^*(1) - E(\infty)}{E(\infty)} \cdot 100\% . \tag{85}$$

The results of our calculations for the factor approximants $E_k^*(\infty)$ and $F_k^*(1)$ are presented in Table 1, together with their errors (77) and (85). As is seen, the method of variable transformation of Sec. 6 is two orders more accurate than the method of power restriction employing restriction (44). The final answer, given by the former method, is $E^*(\infty) = 0.0771$, deviating only by 0.01% from the exact value (73).

8 Pressure of fluctuating membrane

An important class of membranes is formed by those membranes whose constituent molecules can freely move within them. Such membranes are called fluid. The thermal fluctuations of these membranes, at a temperature T, are controlled by their bending rigidity κ . When modeling these membranes, one usually considers them as having a finite length L and an area $A \to \infty$. In order to describe their properties, one, first, assumes

that a membrane is located between the walls of a finite stiffness g. This allows one to resort to perturbation theory in powers of g. But to return to the case of hard walls, one needs to consider the limit $g \to \infty$, which requires to invoke a resummation procedure.

It is convenient to introduce the dimensionless pressure p(g) of a fluctuating membrane, connected with the dimensional pressure P(g) through the relation

$$p(g) \equiv \frac{\kappa L^3}{8T^2} P(g) . \tag{86}$$

The asymptotic behavior of this function, at small $g \to 0$, is represented by the series

$$p_k(g) = \frac{\pi^2}{8g^2} \sum_{n=0}^k a_n g^n . (87)$$

The coefficients of the perturbation series (87) are known only up to the sixth order [31], being

$$a_0 = 1$$
, $a_1 = \frac{1}{4}$, $a_2 = \frac{1}{32}$, $a_3 = 2.176347 \times 10^{-3}$, $a_4 = 0.552721 \times 10^{-4}$, $a_5 = -0.721482 \times 10^{-5}$, $a_6 = -1.777848 \times 10^{-6}$.

We may notice that, up to the second order, the coefficients a_n in pressure (87) are the same as a_n in the ground-state energy (71). The pressure of the membrane, located between hard walls, is given by the limit

$$p(\infty) = \lim_{g \to \infty} p(g) .$$

We shall again find this limit by two methods, by the method of the power restriction (44) and the method of the variable transformation of Sec. 6.

In the direct method of power restriction (44), we find the factor approximants $p_k^*(\infty)$ corresponding to series (87). The approximants p_5^* and p_6^* cannot be defined by this way. And other approximants are

$$p_1^*(\infty) = 0.0193$$
, $p_2^*(\infty) = 0.0232$, $p_3^*(\infty) = 0.3120$, $p_4^*(\infty) = 0.2880$.

The most accurate Monte Carlo calculations for the membrane pressure have been accomplished by Gompper and Kroll [33] giving

$$p_{MC} = 0.0798 \pm 0.0003 \ . \tag{88}$$

As we see, the accuracy of $p_k^*(\infty)$, compared to the Monte Carlo value (88), is rather bad. Now we pass to the more elaborated method of Sec. 6, based on the change of variables prescribed by Eq. (69). The correct choice of the exponent ω_k is very important for achieving a good accuracy of the sought limit $F_k^*(1)$. This exponent is expressed by Eq. (64) through the function (63), for which we take the even factor approximants completely defined in Sec. 2. The series (62), for the considered case, has the same form as in Eq. (78), but with the coefficients

$$c_0 = 1$$
, $c_1 = -\frac{1}{8}$, $c_2 = 0$, $c_3 = 0.64173 \times 10^{-3}$,

$$c_4 = 0.10668 \times 10^{-5}$$
, $c_5 = 0.46253 \times 10^{-5}$, $c_6 = 0.18454 \times 10^{-5}$.

Again, we may notice that the coefficients c_0 , c_1 , and c_2 for the function $\beta_k(g)$, in the case of the membrane, are the same as for series (78) in the case of the string. Constructing the even-order factor approximants $\beta_k^*(g)$ and substituting these into Eq. (64), we find that the sole real exponent ω_k is given by the fourth-order approximant. Thus, we are left with the exponent

$$\omega_k = 1.927 \qquad (k \ge 4) \ . \tag{89}$$

Accomplishing the change of variables (69), we find series (51), for which we construct the factor approximants $F_k^*(z)$. Taking the limit $z \to 1$, we obtain

$$F_4^*(1) = 0.0906$$
, $F_5^*(1) = 0.0898$, $F_6^*(1) = 0.0747$.

Averaging the last two values, we get our final result for the pressure (86) of the fluctuating membrane:

$$p(\infty) = 0.0823. (90)$$

This value is very close to the result [31] of Kastening $p(\infty) = 0.0821$, though it is 3% higher than the Monte Carlo value (88) of Gompper and Kroll [33]. The achieved accuracy is quite good, especially keeping in mind that the method of self-similar factor approximants is much simpler than the numerical method used by Kastening [31] and several orders simpler than the Monte Carlo simulations [33].

9 Conclusion

We have suggested several modifications for constructing self-similar approximants in the frame of the self-similar approximation theory. Two main problems are considered, the problem of interpolation and extrapolation of asymptotic series. The suggested methods are illustrated by examples typical of chemical physics and quantum chemistry.

A special attention is payed to the problem of defining the value of a function at infinity from its expansion at asymptotically small variables. We have designed a new way for constructing the self-similar factor approximants, so that to derive an accurate extrapolation $f(\infty)$ for a function f(g) in the limit of large $g \to \infty$, when only the asymptotic series $f_k(g)$ at small $g \to 0$ are available. We have analyzed and compared two variants of the extrapolation. One of them involves a restriction on the powers of the constructed factor approximants, given by Eq.(44). This variant, however, is not sufficiently accurate. The latter is caused by the fact that the self-similar factor approximants are the most accurate when they are completely defined, by the re-expansion procedure, through the coefficients of the asymptotic series (2). But imposing additional constraints disturbs the self-consistency of the procedure and worsens the accuracy.

The variant of Sec. 6, based on the variable transformation, is essentially more accurate. This is because it does not involve a restriction on powers. Vice versa, it takes into account the additional information on the behavior of the function f(g) when approaching the limit $f(\infty)$. The prescribed change of the variable, not merely tells that $f(\infty)$ is finite, but also describes how f(g) approaches this limit. The accuracy of the method is illustrated by calculating the pressure of fluctuating fluid strings and membranes.

In order to concisely summarize the ideas of the most accurate method, let us briefly delineate its main steps. Suppose we aim at finding the limit $f(\infty)$ of a function f(g), as $g \to \infty$. But what is known for us is only the approximate behavior of the function at asymptotically small $g \to \infty$, where it is approximated by the series $f_k(g)$, and that $f(g) \to const$, as $g \to \infty$. For a given $f_k(g)$, we define the function $\beta_k(g)$ through Eqs. (61) and (62). Then we construct the factor approximants $\beta_k^*(g)$, as in Eq. (63), and define the exponent ω_k by Eq. (64). According to Eq. (69), we make the transformation

$$g_k(z) = \frac{z}{(1-z)^{1/\omega_k}} ,$$

and, as in Eq. (50), introduce $F_k(z) = f_k(g_k(z))$. Constructing the factor approximants $F_k^*(z)$ and taking the limit $z \to 1$, we obtain the values $F_k^*(1)$ approximating the sought-function limit $f(\infty)$. Schematically, all this procedure is represented as the sequence of the following steps:

$$f_k(g) \to \beta_k(g) \to \beta_k^*(g) \to \omega_k \to g_k(z) \to$$

 $\to F_k(z) \to F_k^*(z) \to F_k^*(1) \to f(\infty)$.

We have illustrated the above approach by calculating the pressure of fluid fluctuating membranes. The latter form a rather widespread important class of membranes studied in biology and chemistry [2–6,70]. The asymptotic series for the pressure were derived from Helfrich model [5]. The developed methods can be applied to other systems, where one needs to extrapolate the sought function from the region of asymptotically small variables to their finite values. Moreover, the suggested methods make it even possible to find, with a good accuracy, the limit of the function at infinity. The advantage of the developed methods is their simplicity and high accuracy.

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Table 1

k	$E_k^*(\infty)$	%	$F_k^*(1)$	%
3	0.1500	94.1	0.0593	-23.1
4	0.1370	78.1	0.0935	21.3
5	0.0526	-31.8	0.0926	20.0
6	0.0550	-28.7	0.0829	7.52
7	0.1030	33.4	0.0732	-5.01
8	0.0993	28.8	0.0805	4.36
9	0.0620	-19.6	0.0803	4.17
10	0.0636	-17.5	0.0783	1.49
11	0.0926	20.1	0.0762	-1.24
12	0.0906	17.5	0.0780	1.13
13	0.0662	-14.1	0.0779	1.08
14	0.0674	-12.6	0.0774	0.37
15	0.0882	14.4	0.0768	-0.34
$E^*(\infty)$	0.0778	0.91	0.0771	-0.008

The factor approximants $E_k^*(\infty)$ and $F_k^*(1)$, together with their percentage errors, approximating the ground-state energy $E(\infty)$.